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X-RAY TRANSPORT - II

(BOUND ELECTRON SCATTERING)

KN-65-119(R)   30 March 1965

Kaman
Nuclear
COLORADO SPRINGS, COLORADO
A DIVISION OF KAMAN AIRCRAFT CORPORATION

X-RAY TRANSPORT - II

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F O R E W O R D

This is the second in a series of reports pertaining
to the general problem of x-ray transport through media
in which scattering as well as absorption occurs. In
particular, this report treats the phenomenology of scat-
tering from bound electrons and applies the results to
air.

A B S T R A C T

The phenomenology of generic Compton Scattering, in-
cluding free and bound electrons, is discussed in terms
of the atomic form factor and incoherent scattering
function.

Using Thomas-Fermi data for these functions, average
and differential collision cross sections have been cal-
culated for air for incident photon energies from 0.01 to
1000 kev. An electron binding factor $_a\Sigma$ is defined,
which, when multiplied into Klein-Nishina free electron
collision cross sections, introduces the effect of electron
binding.

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BOUND ELECTRON SCATTERING *

I.   INTRODUCTION

In a previous report[1], Compton scattering was discussed
and reference was made to the influence of electron binding
on scattering of x-rays. This report extends the discussions
in Reference 1 by describing the phenomenology of Compton
bound electron and Rayleigh scattering, introducing a model
for calculating their effects, tabulating data for cross
sections for air, and introducing a factor $_a\Sigma$ called the
Electron Binding Factor (EBF) by which one multiplies Klein-
Nishina collision cross sections per electron $_e\sigma_{KN}$ to obtain
corrected scattering collision cross sections per atom.

II.   SCATTERING PHENOMENOLOGY

Compton effect discussions make clear the conservation
of relativistic energy and momentum and the shift to longer
wavelengths of scattered photons in a manner dependent on
scattering angle θ but independent of the scatterer atomic
number Z.   It is true that Compton's description of the
event[2] is independent of Z, but the generic phenomenon usually
referred to as Compton scattering (which includes actual per-
formance of an experiment) does depend on Z. This dependence
is due to binding of electrons in atoms whereas Compton's
discussion is for free electrons.

A.   Compton (Incoherent) Scattering

The probability of a free electron scattering a photon
$h\nu_0$ into a solid angle $d\Omega$ at θ is given by the Klein-Nishina
equation

$$d(_e\sigma_{KN}) = (r_o^2/2) \left[\frac{1}{1 + \alpha(1 - \cos\theta)} \right]^2 (1 + \cos^2\theta)$$

$$\left\{ 1 + \frac{\alpha^2 (1 - \cos\theta)^2}{(1 + \cos^2\theta)[1 + \alpha(1 - \cos\theta)]} \right\} d\Omega. \tag{1}$$

$$\equiv g(\alpha, \theta)d\Omega$$

where r_o = electron radius, $\alpha = h\nu_o/m_o c^2$, and m_o = electron rest mass.

The incoherent scattering probability may be considered the product of probabilities of two mutually exclusive events: first, that the photon is scattered into $d\Omega$ at θ with a transfer of momentum $\vec{q}$ to the electron; and, second, that after receiving the momentum, the electron will absorb energy and recoil. The first probability is given by $g(\alpha, \theta)$, and for a free electron (transferred momentum >> initial electron momentum) the second probability is unity. If the electron were in an atom, then for incident photon energies approaching binding energies, B_e, the probability of the electron's absorbing sufficient energy to recoil free of the atom decreases. The electron is more likely only to be raised to another bound level. This may be described by a probability function called the incoherent scattering function $S(\vec{q},Z) \equiv S(\alpha,\theta,Z)$ which decreases from one to zero as $\vec{q}$ decreases (or Z increases), and in which the binding energy is given in terms of Z.

Compton scattering per atom, including that from bound electrons, then may be described by

$$d_a\sigma_{incoh} = Zg(\alpha,\theta)\ S(\alpha,\theta,Z)d\Omega \qquad (2)$$

with an average incoherent collision cross section per atom,

$$a^{\sigma_{incoh}} = \int Zg(\alpha,\theta)\ S(\alpha,\theta,Z)\ d\Omega. \qquad (3)$$

Another consequence of electron binding is that the shift to longer wavelength of the scattered photon is less than the shift due to scattering from a free electron.

For a free electron it is given by

$$\lambda' - \lambda_o = (h/m_oc)\ (1 - \cos\theta) \qquad (4)$$

but for a bound electron it is

$$\lambda'' - \lambda_o = (h/m_oc)\ (1 - \cos\theta) - \lambda_o^2\ D \qquad (5)$$

where $D = b\ B_e/hc$ in which[3] $b \approx 1$ and B_e = binding energy.

The effect of this "defect in the Compton shift" on the transport of photons in air is presently being investigated and will be included in a future Kaman Nuclear X-Ray transport document.

B. Rayleigh (Coherent) Scattering

When incident photon energy is low enough, compared to the electron's binding energy, so that insufficient energy is transferred even for excitation of the electron to a higher bound level the atom as a whole absorbs the momentum, the

scattered photon wavelength is not shifted, and scattering from all electrons in an atom is Rayleigh (coherent) scattering. For the most tightly bound electrons ($h\nu_o \ll B_e$) the probability per electron of scattering into $d\Omega$ at θ is the classical Thomson (coherent) scattering, where

$$d_e\sigma_{Thom} = (r_o^2/2) (1 + \cos^2 \theta)d\Omega \equiv h(\theta)d\Omega. \qquad (6)$$

In a manner analogous to that for Compton scattering we consider Rayleigh scattering as made up of two probabilities. The first is the Thomson function, $h(\theta)$, and the second is a function of the atomic form factor which describes the relative degree of electron binding in terms of the incident photon energy and Z of the scatterer. This second factor is the probability that the Z electrons will absorb momentum $\vec{q}$ with no increase in energy. It describes the qualitative concept that as $h\nu_o$ increases the electrons of the atom appear to the incoming photon to be less tightly bound, until in the high energy limit the electrons are considered to be free. Thus the function varies from one (tight binding) to zero (free) as the incident energy increases (or Z decreases).

By incorporating this form factor function into the Thomson scattering equation, then, one can describe Rayleigh scattering per atom by

$$d_a\sigma_{coh} = h(\theta)[F(\alpha,\theta,Z)]^2 d\Omega, \qquad (7)$$

with an average coherent collision cross section per atom

$$a\sigma_{coh} = \int h(\theta)[F(\alpha,\theta,Z)]^2 d\Omega. \qquad (8)$$

C. Total Scattering

Total scattering p⁻ atom then is given by the probability of scattering into $d\Omega$ at θ;

$$d_a\sigma_T = \left\{ Zg(\alpha,\theta)S(\alpha,\theta,Z) + h(\theta) \left[F(\alpha,\theta,Z)\right]^2 \right\} d\Omega$$

$$\equiv f_a (\alpha,\theta,Z)d\Omega. \tag{9}$$

The average total collision cross section per atom for scattering then is

$$_a\sigma_T = \int f_a (\alpha,\theta,Z)d\Omega. \tag{10}$$

From the discussions above in Sections II.A and II.B we see that S and F are related, F being the more fundamental. They compete and there is some energy region where their contributions to the total cross section are comparable. Their relationship is discussed below in Section IV.

Scattering is influenced by anomalous dispersion which occurs near absorption edges of materials. This effect which has been neglected here, should be considered when for a particular problem a material and photon energy are selected.

III. ATOMIC FORM FACTOR

For an atom with atomic number Z the atomic form factor is defined as the matrix element

$$F(\alpha,\theta,Z) - F(\vec{q},Z) = \langle o| \sum_{j=1}^{Z} e^{i\vec{q} \cdot r_j /\hbar}| o \rangle , \tag{11}$$

where o represents the atomic ground state and $\vec{r}_j$ is the vector from the nucleus to the jth electron. $F(\alpha,\theta,Z)$ represents the ratio of the <u>amplitude</u> of the coherent scattering from an atom to that from a free electron. The scattering <u>intensity</u> ratio is given by F^2.

Various models used for calculating F have been reported and reviews of the literature are available.[4] We select the Thomas-Fermi model[5,6], which represents a qualitative average of the others, describing F as a function of the variable[5]

$$u = 2(137/Z^{1/3})\ \alpha\ \sin\ (\theta/2). \qquad (12)$$

Values for F/Z from Nelms and Oppenheim[4] are plotted in Reference 1.

IV. INCOHERENT SCATTERING FUNCTION

This function is the probability that an atom is raised to an excited state as a result of a transfer of momentum $\vec{q}$ and is given by the sum over excited states of the squares of the generalized form factors, divided by Z, or

$$S(\alpha,\theta,Z) = S(\vec{q},Z) = \frac{1}{Z}\sum_{\epsilon\neq o}\left[\langle\epsilon|\sum_{j=1}^{Z}e^{i\vec{q}\cdot\vec{r}_j/h}|o\rangle\right]^2, \qquad (13)$$

in which ϵ represents excited states. The relation between the incoherent scattering function, S, and the coherent scattering function, F^2/Z, is now evident. The coherent scattering function is the ground state term in the summation over states shown in Equation (13). The matrix element

between ground states involves no energy change, thus <u>coherence</u>, while the remainder of the summation (over the excited states) involves terms implying energy shifts, the <u>incoherent</u> part of the scattering.

Thomas-Fermi data from Grodstein[7] are plotted in Reference (1) for $S = S(v)$, where

$$v = (2/3) \ (137/Z^{2/3}) \ \alpha \ \sin \ (\theta/2). \tag{14}$$

V. RESULTS OF COMPUTATIONS

Computations were performed with programs written in Fortran for Control Data 1604 and 3400 computers.

A steepest descent curve fit program was developed and the Thomas-Fermi data for S and F^2/Z were fitted to empirical functions to within 10%. These were used for computing $\int gs d\Omega$ and $\int h(F^2/Z)d\Omega$ and results compared to those obtained using the data only. Differences of up to an order of magnitude were observed. This is because integration over θ from zero to π results in integration over u or v from zero to some restricted value depending on α and Z resulting in integration over restricted values of the empirical functions for S or F^2/Z so that errors are not averaged but may accumulate.

A. Incoherent Scattering

Using the data of Grodstein[7] in Equation (3) we get $_a\sigma_{incoh}$ for air which is listed in Table I and plotted in Figure 1. Photoelectric absorption cross sections σ^{PE} have been included for comparison. The differential collision cross section $d(_a\sigma_{incoh})/c\theta$ for air at three different energies is shown in Figures (2), (3), and (4). Cross sections for materials other than air are published in Part III of this series of reports[8].

TABLE 7

INCOHERENT, COHERENT, AND TOTAL SCATTERING
AVERAGE COLLISION CROSS SECTIONS
AND ELECTRON BINDING FACTORS FOR AIR

| $h\nu_0$ (kev)	$_a\sigma_{incoh}$ (cm^2/atom)	$_a\sigma_{coh}$ (cm^2/atom)	$_a\sigma_T$ (cm^2/atom)	$_a\Sigma$
0.1	1.580-025	3.435-023	3.451-023	5.190+001
.2	3.005-025	3.365-023	3.395-023	5.108+001
.4	5.435-025	3.227-023	3.282-023	4.941+001
.6	7.489-025	3.093-023	3.168-023	4.773+001
.8	9.277-025	2.962-023	3.055-023	4.606+001
1.0	1.086-024	2.832-023	2.941-023	4.438+001
2	1.683-024	2.197-023	2.365-023	3.583+001
4	2.438-024	1.376-023	1.620-023	2.473+001
6	2.915-024	9.330-024	1.225-023	1.884+001
8	3.232-024	6.736-024	9.968-024	1.545+001
10	3.451-024	5.072-024	8.524-024	1.331+001
20	3.914-024	1.905-024	5.819-024	9.415+000
40	3.927-024	6.292-025	4.556-024	7.872+000
60	3.768-024	3.152-025	4.083-024	7.483+000
80	3.602-024	1.878-025	3.790-024	7.326-000
100	3.449-024	1.240-025	3.573-024	7.252+000
200	2.890-024	3.270-026	2.923-024	7.190-000
400	2.278-024	8.421-027	2.287-024	7.220-000
600	1.932-024	3.851-027	1.935-024	7.235+000
800	1.700-024	2.578-027	1.702-024	7.244+000
1000	1.529-024	1.915-027	1.531-024	7.250+000
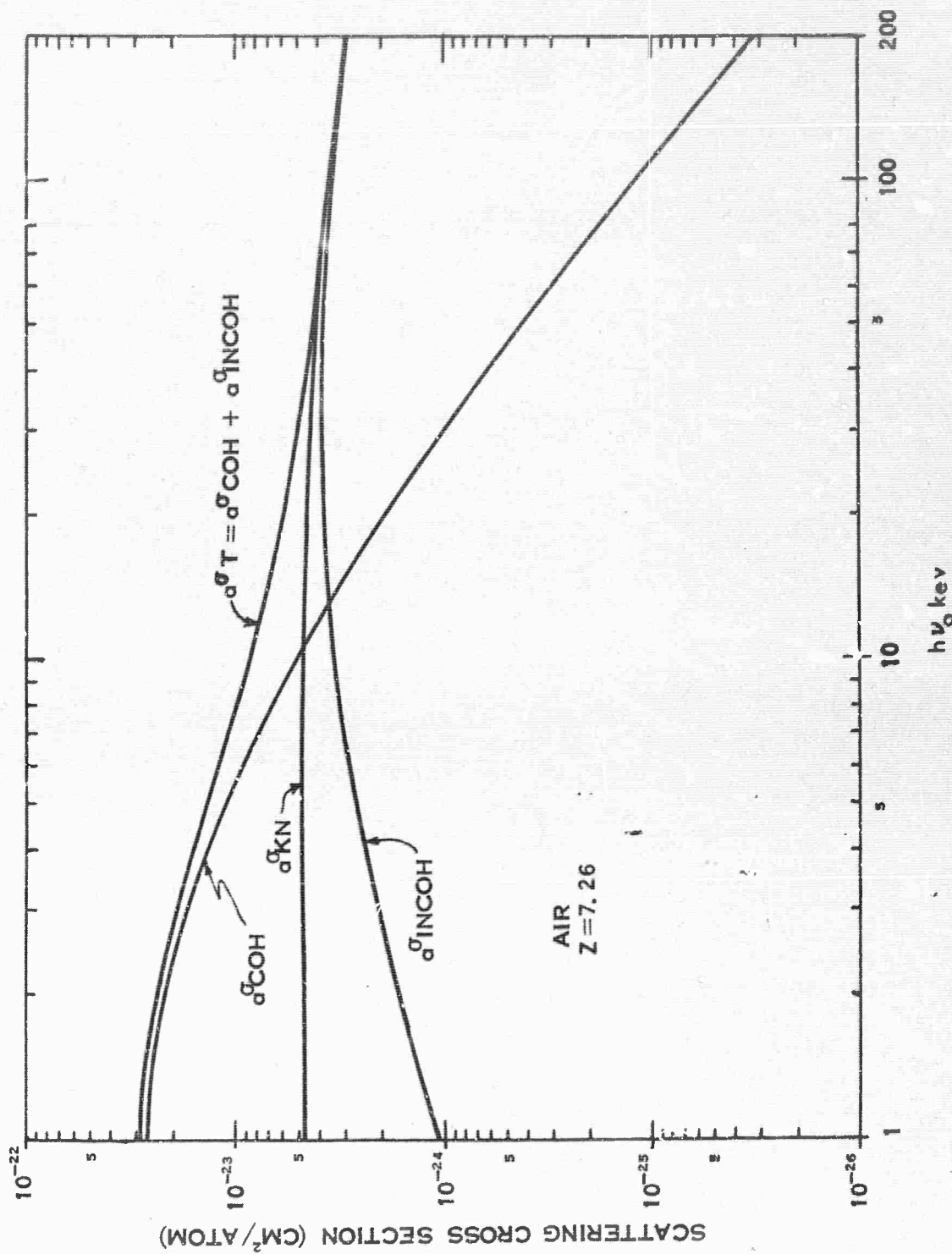
FIGURE (1)

$\dfrac{d\sigma}{d\theta}$ IN 10^{-24} CM^2/RADIAN–ATOM

AIR
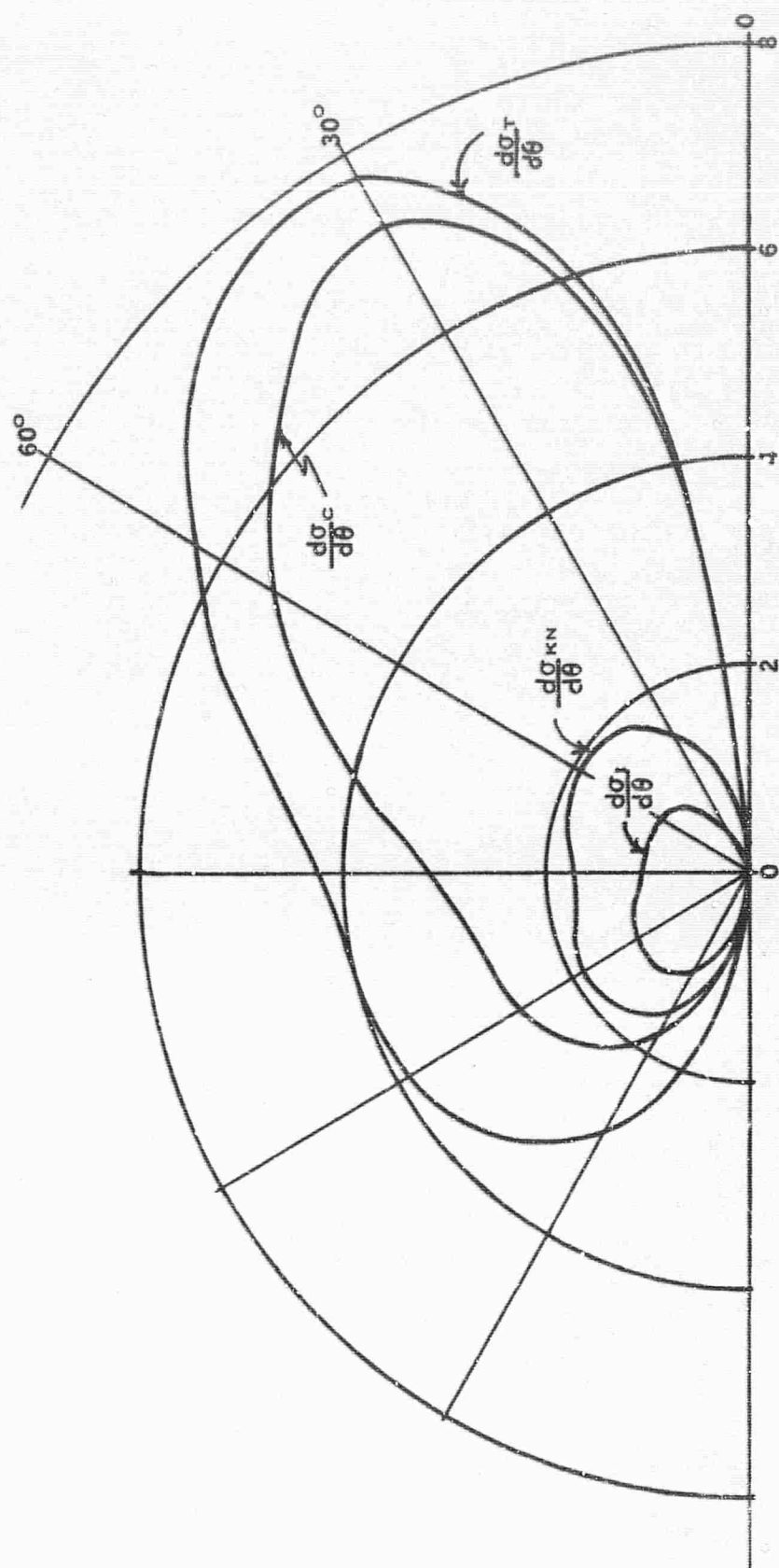
Z = 7.26

hν_0 = 5 kev
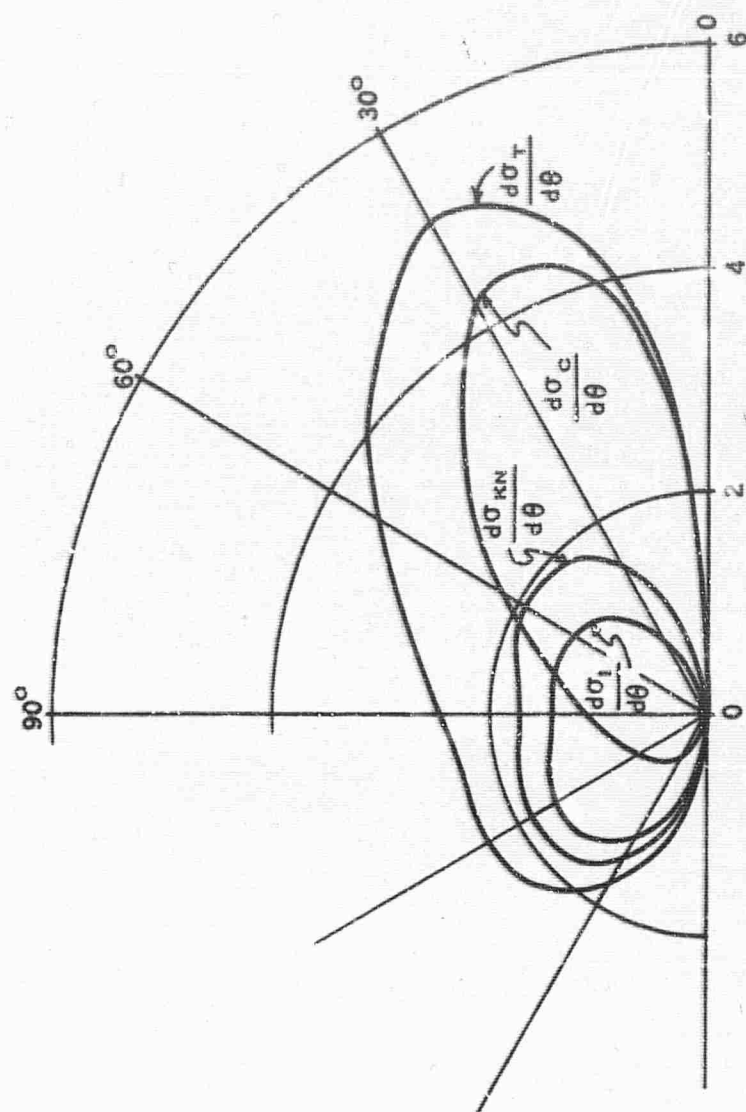
FIGURE (2)

$$\frac{d\sigma}{d\theta} \quad \text{IN } 10^{-24} \text{ CM}^2/\text{RADIAN} - \text{ATOM}$$

AIR
$Z = 7.26$
$h\nu_0 = 10$ kev

FIGURE (3)

$$\frac{d\sigma}{d\theta} \text{ IN } 10^{-24} \text{ CM}^2 / \text{RADIAN} - \text{ATOM}$$
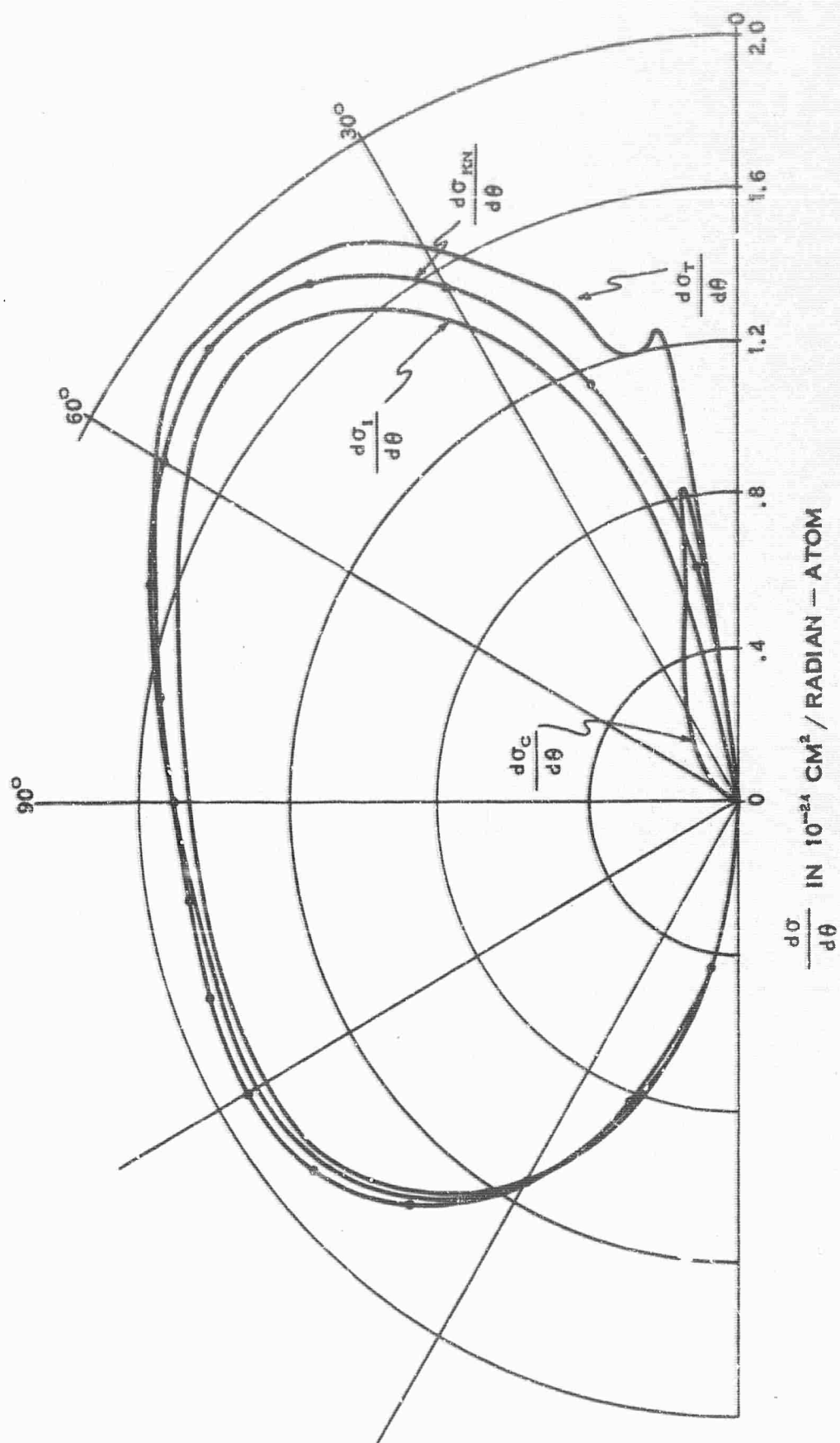
AIR
$Z = 7.26$
$h\nu_0 = 50$ kev

FIGURE (4)

B. Coherent Scattering

Using the data of Nelms and Oppenheim[4] in Equation (8) we get $_a\sigma_{coh}$ for air which is listed in Table I and plotted in Figure 1, and $d(_a\sigma_{coh})/d\theta$ is shown in Figures (2), (3), and (4). See Reference 8 for materials other than air.

C. Total Scattering

From Equation (1) $_a\sigma_T$ for air was calculated, listed in Table I, and plotted in Figure 1. Figures (2), (3), and (4) show $d(_a\sigma_T)/d\theta$. See Reference 8 for materials other than air.

D. Electron Binding Factor

Klein-Nishina free electron collision cross sections per electron $_e\sigma_{KN}$ are generally available; therefore, it is convenient to define a quantity, here called the electron binding factor (EBF), for different materials which may be multiplied into $_e\sigma_{KN}$ to account for electron binding and give the total average collision cross section per atom $_a\sigma_T$.

Equation (1) may be written

$$a\sigma_T = \int (ZS + F^2h/g)gd\Omega = \overline{(ZS + F^2h/g)} \int gd\Omega = {}_a\Sigma\, _e\sigma_{KN} \qquad (16)$$

where $_a\Sigma$ is the EBF defined by

$$a\Sigma = \frac{\int(ZS + F^2h/g)gd\Omega}{\int gd\Omega} . \qquad (17)$$

EBF values for air are listed in Table I and plotted in Figure 5. Values for media other than air are listed in Reference 8.
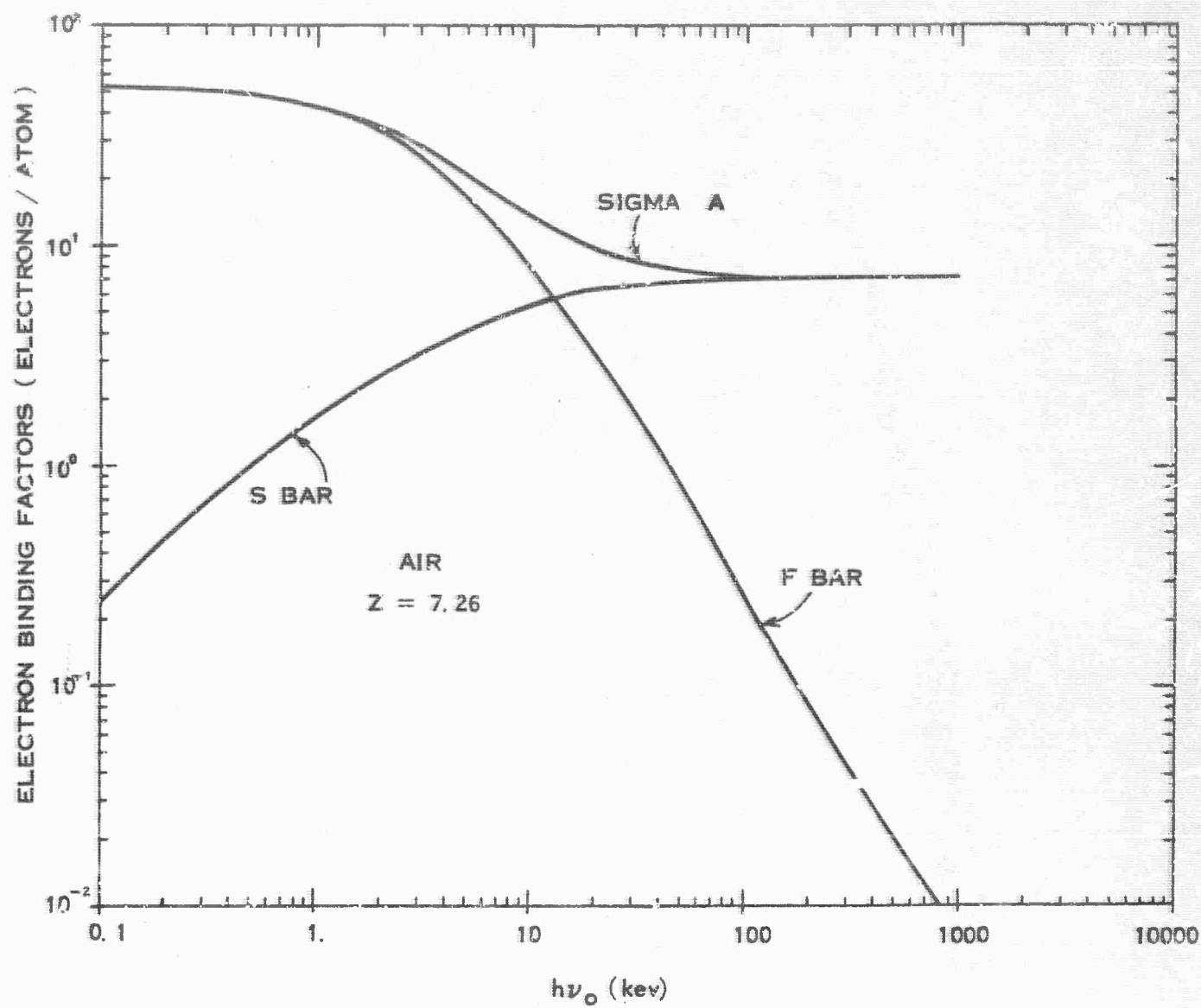
FIGURE (5)

VI   DISCUSSION OF RESULTS

Figure (1) shows that for $h\nu_0 > 30$ kev the Klein-Nishina
cross sections are close to those calculated using the bound
electron correction, but at lower energies the two differ by
up to an order of magnitude.

The differential cross sections depict the probability
of scattering into an angle $d\theta$ at θ. Figures (2), (3), and
(4) which include Klein-Nishina values, demonstrate the con-
tributions of incoherent and coherent to total scattering,
including electron binding, and compare them with that ex-
pected from the free electron assumption of Klein and Nishina.

Footnotes

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3. G. Wentzel, Z. Physik $\underline{43}$, 1,779 (1927); P.A. Ross and P. Kirkpatrick, Phys. Rev. $\underline{45}$, 223 (1934); F. Bloch, Phys. Rev. $\underline{46}$, 674 (1934).

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